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**A journal devoted to experimental and theoretical research  
involving problems of both a chemical and a physical nature**

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*Editors*

**ROBIN M. HOCHSTRASSER/G. LUDWIG HOFACKER**

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# CHEMICAL PHYSICS

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- Casida, M.E. and D.P. Chong, Contribution of correlation and relaxation to generalized overlaps for outer valence ionization. Chem. Phys. 133 (1989) 47. Erratum 136 (1989) 489
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- Garrett, B.C., T. Joseph, T.N. Truong and D.G. Truhlar, Application of the large-curvature tunneling approximation to polyatomic molecules: abstraction of H or D by methyl radical 136 (1989) 271
- Garrett, B.C., T. Joseph, T.N. Truong and D.G. Truhlar, Application of the large-curvature tunneling approximation to polyatomic molecules: abstraction of H or D by methyl radical. Chem. Phys. 136 (1989) 271. Erratum 140 (1990) 207
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- González, M., A. Aguilar and M. Gilibert, Dynamics of the  $O^+(^4S) + H_2(X^1\Sigma_g^+) \rightarrow OH^+ + H$  ion-molecule reaction and some of its isotopic variants ( $D_2$  and  $HD$ ). II. Quasiclassical trajectory study in the range of relative energies 0.25-6.30 eV 131 (1989) 347
- González, M., A. Aguilar and M. Gilibert, Dynamics of the  $O^+(^4S) + H_2(X^1\Sigma_g^+) \rightarrow OH^+ + H$  ion-molecule reaction and some of its isotopic variants ( $D_2$  and  $HD$ ). II. Quasiclassical trajectory study in the range of relative energies 0.25-6.30 eV. Chem. Phys. 131 (1989) 347. Erratum 133 (1989) 172
- González, M., A. Aguilar and R. Sayós, Low energy dynamics, isotopic effects and detailed microscopic reaction mechanism of the ion-molecule reaction  $N^+(^3P) + H_2 \rightarrow NH^+ + H$  132 (1989) 137
- González, M. and A. Aguilar, On the reliability of a reasonable single surface treatment of the reaction  $C^+(^2P) + H_2(X^1\Sigma_g^+) \rightarrow CH^+ + H$  at relative energies from the threshold region up to 2.0 eV 132 (1989) 443
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- Guimon, C., S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo, HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of  $\text{CN}_2\text{H}_2$  energy hypersurface 138 (1989) 157
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- Gutmann, M., P.-F. Schönzart and G. Hohlneicher, High-resolution one- and two-photon spectroscopy of matrix-isolated molecules. II. Investigations on naphthalene and octadeuteronaphthalene 140 (1990) 107

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- Hirao, K., see H. Wasada 138 (1989) 277
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- Kosmas, A.M. and R.J. Williams, A classical trajectory study of the  $\text{O}(^3\text{P}) + \text{I}_2$  reaction 140 (1990) 413
- Kosugi, N., H. Kondoh, H. Tajima and H. Kuroda, Cu K-edge XANES of  $(\text{La}_{1-x}\text{Sr}_x)_2\text{CuO}_4$ ,  $\text{YBa}_2\text{Cu}_3\text{O}_y$ , and related Cu oxides. Valence, structure and final-state effects on  $1s-4p\pi$  and  $1s-4p\sigma$  absorption 135 (1989) 149
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- Kukolich, S.G. and D.J. Pauley, Centrifugal distortion analysis for the bent isomer of  $\text{N}_2\text{O}-\text{HF}$ . Chem. Phys. 131 (1989) 403. Erratum 135 (1989) 161
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- Umemoto, H., J. Kikuma, A. Masaki, T. Takayanagi and S. Sato, The intramultiplet mixing of  $\text{Zn}(4^3\text{P}_J)$  by collisions with rare gas atoms. Chem. Phys. 134 (1989) 193. Erratum 137 (1989) 427
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- Ab initio calculations of the structure and infrared spectrum of PO<sub>2</sub>, P<sub>2</sub>O and P<sub>4</sub>O, S.A. Jarrett-Sprague, I.H. Hillier and I.R. Gould 140 (1990) 27
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- Quantum treatment of the optical spectra and the initial electron transfer process within the reaction center of *Rhodopseudomonas viridis*, P.O.J. Scherer and S.F. Fischer 131 (1989) 115
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- Electronic bath theory: multi-orbital primary zone, H.K. McDowell 132 (1989) 59
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- Fractal analysis of Brownian dynamics simulations of diffusion-controlled reactions, M.A. López-Quintela, M.C. Buján-Núñez and J.C. Pérez-Moure 132 (1989) 83
- The intramolecular fluorescence quenching in cylindrical micelles. II, M. Van der Auweraer, S. Reekmans, N. Boens and F.C. De Schryver 132 (1989) 91
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- Binding energies and structures of  $NH_3$  clusters, J.C. Greer, R. Ahlrichs and I.V. Hertel 133 (1989) 191
- Electron impact direct dissociation processes of vibrationally excited  $H_2$  molecules to excited atomic hydrogen  $H^*(n=1-5)$ . I. Cross sections, R. Celiberto, M. Cacciatore, M. Capitelli and C. Gorse 133 (1989) 355
- Electron impact direct dissociation processes of vibrationally excited  $H_2$  molecules to excited atomic hydrogen  $H^*(n=1-5)$ . II. Translational energy distribution functions of dissociation products, R. Celiberto, M. Cacciatore and M. Capitelli 133 (1989) 369
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- Lennard-Jones fluid between adiabatically moved interacting walls, S.-B. Zhu and G.W. Robinson 134 (1989) 1
- Trajectory calculations of the capture rate coefficients for the  $D_3^+ + C_6F_6$  reactions, I. Mendaš and P. Milutinović 134 (1989) 47
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- Energy distributions from decomposition of a complex  $H_2O \rightarrow OH + H$  on a simplified potential energy surface, as a function of total angular momentum: comparison between classical trajectories and an RRKM-type statistical simulation, G. Nyman, K. Rynefors and L. Homlid 134 (1989) 355
- Charge fluctuations in high- $T_c$  superconducting cuprates: a reformulation of the "symmetry dilemma" of the mean-field approximation, M.C. Böhm, G. Bubeck and A.M. Oleś 135 (1989) 27
- The influence of collisions on laser absorption spectra of  $SF_6$ , G.D. Billing and D.C. Clary 135 (1989) 91
- The Sixl-Higelin salicylideneaniline molecular switch revisited, P. Sautet and C. Joachim 135 (1989) 99
- Group theoretical statistical mechanics of nematogenic and cholesteric liquid crystals, M.W. Evans 135 (1989) 187
- Study of molecular phase space structure through families of periodic orbits, S.C. Farantos, M. Founargiotakis and C. Polymilis 135 (1989) 347
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- Magnetic and spin effects in recombination and disproportionation of radicals generated under photolysis of deoxybenzoins in micelles, V.F. Tarasov, I.A. Shkrob, E.N. Step and A.L. Buchachenko 135 (1989) 391
- Semi-local pseudopotential calculations for the adiabatic potentials of alkali-neon systems, E. Czuchaj, F. Rebertus, H. Stoll and H. Preuss 136 (1989) 79
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- Ab initio calculations of electric field gradient for the B...H-Cl dimers: B=CO, HCN,  $H_2O$ ,  $H_2S$ ,  $C_2H_2$ ,  $C_2H_4$ ,  $NH_3$ ,  $PH_3$  and  $CH_3CN$ , W.B. De Almeida and A. Hinchliffe 137 (1989) 143
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- Transition moment directions and molecular structure of some *p*-cyano-N,N-dimethylaniline derivatives, J. Herbich, K. Rotkiewicz, J. Waluk, B. Andresen and E.W. Thulstrup 138 (1989) 105
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- An MNDO calculational study of selected oxazine, thiazine and oxazone dyes, G.J. Blanchard 138 (1989) 365
- The role of state specificity in unimolecular rate theory, W.L. Hase, S.-W. Cho, D. Lu and K.N. Swamy 139 (1989) 1
- Van der Waals bound states and intermolecular bend-stretch coupling in Ne- $C_2H_4$  and Ar-tetrazine, A.R. Tiller and D.C. Clary 139 (1989) 67
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- Quadratic hyperpolarisability of sulfur-containing systems, M. Barzoukas, D. Josse, J. Zyss, P. Gordon and J.O. Morley 139 (1989) 359
- The breakdown of the isolated binary collision hypothesis for near-resonant VV processes in liquid argon, J.J. Andrew, A.P. Harriss, D.C. McDermott, H.T. Williams, P.A. Madden and C.J.S.M. Simpson 139 (1989) 369
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- The use of the isokinetic relationship and molecular mechanics to investigate molecular interactions in inclusion complexes of cyclodextrins, W. Linert, L. Han and I. Lukovitz 139 (1989) 441
- Dissipative effects on highly excited quantum states of a model two-degree-of-freedom system, R. Olender and E. Pollak 139 (1989) 471
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- Rate constants and rotational relaxation times for  $N_2$  in argon: theory and experiment, A.E. Belikov, A.I. Burshtein, S.V. Dolgushev, A.V. Storozhev, M.L. Strelakov, G.I. Sukhinin and R.G. Sharafutdinov 139 (1989) 239
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## Experimental

### *Magnetic resonances*

- Low-field CIDNP manifestation of the minor recombination channel via the triplet state of radical pairs, E.C. Korolenko, N.V. Shokhirev, K.M. Salikhov and R.Z. Sagdeev 131 (1989) 315
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- A quasi-neutral triplet state of TCNQ in phenazine/TCNQ and fluorene/TCNQ CT crystals, D. Gundel, J. Frick, J. Krzystek, H. Sixl, J.U. von Schütz and H.C. Wolf 132 (1989) 363
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- Muon level crossing resonance study of radical formation in allylbenzene, styrene and toluene, K. Venkateswaran, M.V. Barnabas, Z. Wu, J.M. Stadlbauer, B.W. Ng and D.C. Walker 137 (1989) 239
- Spin-locking in concentration-narrowed OD ESR spectra, A.V. Koptug, V.O. Saik, O.A. Anisimov and Yu.N. Molin 138 (1989) 173
- Methyl tunnelling in tiglic acid and 2-methyl-2-butene, A.J. Horsewill, R.M. Green and A.M. Alsanoosi 138 (1989) 179
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- Kinetics of nuclear polarization in the geminate recombination of biradicals, Yu.P. Tsentalovich, A.V. Yurkovskaya, R.Z. Sagdeev, A.A. Obynochny, P.A. Purtov and A.A. Shargorodsky 139 (1989) 307
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- Intermolecular H-tunneling in a solid state photoreaction promoted by distinct low-energy nuclear fluctuation modes, B. Prass, J.P. Colpa and D. Stehlik 136 (1989) 187
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- other large*
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### *-dimers*

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- The linear and T-shaped isomers of  $C_2H_2-HCN$ : vibrational dynamics from infrared spectroscopy and ab initio theory, P.A. Block, K.W. Jucks, L.G. Pedersen and R.E. Miller 139 (1989) 15
- Van der Waals bound states and intermolecular bend-stretch coupling in  $Ne-C_2H_4$  and Ar-tetrazine, A.R. Tiller and D.C. Clary 139 (1989) 67



- Mode selective control of unimolecular dissociations: survey and model simulations for  $\text{HDO} \rightarrow \text{H} + \text{DO}$ ,  $\text{D} + \text{HO}$ , B. Hartke, J. Manz and J. Mathis 139 (1989) 123
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- A theoretical study of methoxy group rotation in anisole, M.A. Vincent and I.H. Hillier 140 (1990) 35
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- CARS measurements of intra-mode V-V exchange rate constants of nitrogen, S.I. Valyansky, K.A. Vereschagin, A.Yu. Volkov, V.V. Smirnov and V.I. Fabelinsky 140 (1990) 59
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- Electronic structure and states*
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- Photoelectron and ab initio configuration interaction studies of  $(\text{NSF})_3$  and  $(\text{NSF})_4$ ; trends, and geometric and electronic structures in the  $(\text{NSF})_x$  ( $x=1,2,3$ , and 4) series, M.H. Palmer, R.T. Oakley and N.P.C. Westwood 131 (1989) 255
- Theoretical interpretation of the electroabsorption spectrum of the anthracene crystal, P. Petelenz and V.H. Smith Jr. 131 (1989) 409
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- The possibility of molecular switching: theoretical study of  $[(\text{NH}_3)_5\text{Ru}-4,4'\text{-bipy}-\text{Ru}(\text{NH}_3)_5]^{5+}$ , S. Woitellier, J.P. Launay and C. Joachim 131 (1989) 481
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- Formation of the low-lying electronic states of CrO in highly exothermic reactive oxidation. Assessment of new states and partial resolution of previous observations, T.C. Devore and J.L. Gole 133 (1989) 95
- The electronic states of benzene and the azines. I. The parent compound benzene. Correlation of vacuum UV and electron scattering data with ab initio CI studies, M.H. Palmer and I.C. Walker 133 (1989) 113
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- The treatment of electron correlation in aperiodic systems. II. Applications to poly(Li<sub>2</sub>H<sub>2</sub>) and poly(acetylene, carbyne) chains, C.-M. Liegener, A.K. Bakhshi, A. Sutjianto and P. Otto 133 (1989) 177
- Band structure of charge transfer excitons in anthracene, P. Petelenz 133 (1989) 199
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- Semi-empirical determination of the long-range molecular states dissociating to C(<sup>3</sup>P<sub>J</sub>) + O(<sup>3</sup>P<sub>J</sub>), B. Bussery, M.E. Rosenkrantz, D.D. Konowalow and M. Aubert-Frécon 134 (1989) 7
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- Symmetry, selection rules, and energy levels of Pr<sup>3+</sup>:Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub>, J.B. Gruber, M.E. Hills, R.M. MacFarlane, C.A. Morrison and G.A. Turner 134 (1989) 241
- Theoretical study of the correlation effects in the photoelectron spectrum of bis(π-allyl)nickel, P. Decleva, G. Fronzoni and A. Lisini 134 (1989) 307
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- Sulfochloration of trifluoromethane. Theoretical study of the trifluoromethane sulfonyl radical, D. Gonbeau, M.F. Guimon, S. Duplantier, J. Ollivier and G. Pfister-Guillouzo 135 (1989) 85
- The Sixl-Higelin salicylideneaniline molecular switch revisited, P. Sautet and C. Joachim 135 (1989) 99
- Cu K-edge XANES of  $(La_{1-x}Sr_x)_2CuO_4$ ,  $YBa_2Cu_3O_y$  and related Cu oxides. Valence, structure and final-state effects on  $1s-4p\pi$  and  $1s-4p\sigma$  absorption, N. Kosugi, H. Kondoh, H. Tajima and H. Kuroda 135 (1989) 149
- $NO_2$  radical spectroscopy: vibrational frequencies, dipole moment, and the energy difference between the bent and linear stationary points on the ground state potential surface, Y. Xie, R.D. Davy, B.F. Yates, C.P. Blahous III, Y. Yamaguchi and H.F. Schaefer III 135 (1989) 179
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- Jahn-Teller effect for the  $4s^2(^1S_0) \rightarrow 4s4p(^1P_1)$  resonance transition of zinc in rare gas matrices from magnetic circular dichroism measurements, B. Hoffmann-Millack, A. Klein, H. Lagier, B. Maid and J. Hormes 136 (1989) 453
- MRD CI calculations on the radiative lifetime of the  $A^2\Delta$  state of CH, G. Theodorakopoulos, I.D. Petsalakis, R.J. Buenker and M. Honigmann 137 (1989) 137
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- The valence orbital momentum distributions and binding energy spectra of dimethyl ether by electron momentum spectroscopy: an investigation of the methyl inductive effect, S.A.C. Clark, A.O. Bawagan and C.E. Brion 137 (1989) 407
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- Semi-local pseudopotential calculations for the potential energies of the  $\text{CaHe}$  and  $\text{CaNe}$  systems, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 138 (1989) 303
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- The influence of singlet-triplet transitions on non-stationary kinetics of radical recombination in homogeneous solutions. II. Numerical case studies, E.B. Krissinel', N.V. Shokhirev and K.M. Salikhov 137 (1989) 207
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- Electron delocalization in trinuclear iron-sulfur clusters from *Desulfovibrio gigas*, S.A. Borshch and L.F. Chibotaru 135 (1989) 375
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- Muon level crossing resonance study of radical formation in allylbenzene, styrene and toluene, K. Venkateswaran, M.V. Barnabas, Z. Wu, J.M. Stadlbauer, B.W. Ng and D.C. Walker 137 (1989) 239
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- Many-body effects in ion-water interactions:  $\text{Fe}^{3+}$  in water, L.A. Curtiss, J.W. Halley and J. Hautman 133 (1989) 89
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- Diode laser kinetic measurements of vibrational, rotational and translational temperatures of CO in CO<sub>2</sub> laser-excited SF<sub>6</sub>, K. Sugawara, T. Nakanaga, H. Takeo and C. Matsumura 135 (1989) 301
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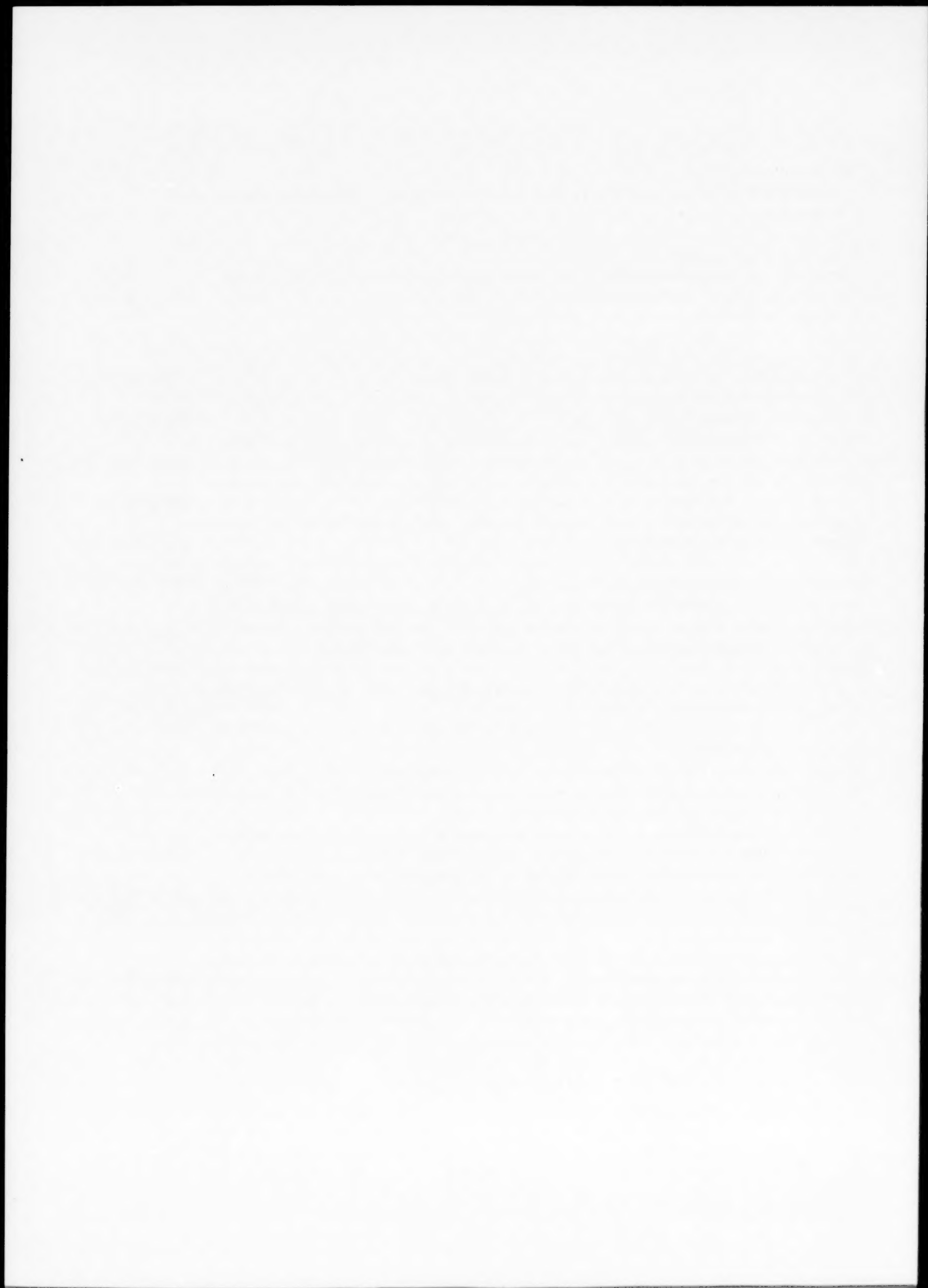
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